

Carbonic acid, but-3-yn-1-yl nonyl ester

Inchi:	InChI=1S/C14H24O3/c1-3-5-7-8-9-10-11-13-17-14(15)16-12-6-4-2/h2H,3,5-13H2,1H3
InchiKey:	KBQICJNJWOXOSG-UHFFFAOYSA-N
Formula:	C14H24O3
SMILES:	C#CCCOC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	240.34

Physical Properties

Property code	Value	Unit	Source
gf	-48.85	kJ/mol	Joback Method
hf	-417.41	kJ/mol	Joback Method
hfus	38.97	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.913		Crippen Method
mvol	212.830	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	608.55	K	Joback Method
tc	784.66	K	Joback Method
tf	388.90	K	Joback Method
vc	0.824	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.74	J/mol×K	608.55	Joback Method
cpg	568.45	J/mol×K	637.90	Joback Method
cpg	583.49	J/mol×K	667.25	Joback Method
cpg	597.87	J/mol×K	696.61	Joback Method
cpg	611.61	J/mol×K	725.96	Joback Method
cpg	624.70	J/mol×K	755.31	Joback Method
cpg	637.15	J/mol×K	784.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383176&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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